Finite Difference EM modeling efforts of COMPASS

Presenter: John R. Cary

COMPASS Review 21Apr09

- Physics Goals
- Basics
- Algorithmic accomplishments
- Physics accomplishments
- Interactions with CETs
- VORPAL community
- Future directions
- Publications

Acknowledgements: T. Austin, G. I. Bell, D. L. Bruhwiler, R. S. Busby, M. Carey, J. Carlsson, J. R. Cary, Y. Choi, B. M. Cowan, D. A. Dimitrov, A. Hakim, J. Loverich, S. Mahalingam, P. Messmer, P. J. Mullowney, C. Nieter, K. Paul, C. Roark, S. W. Sides, N. D. Sizemore, D. N. Smithe, P. H. Stoltz, S. A. Veitzer, D. J. Wade-Stein, G. R. Werner, M. Wrobel, N. Xiang, C. D. Zhou

Electromagnetic modeling goals are

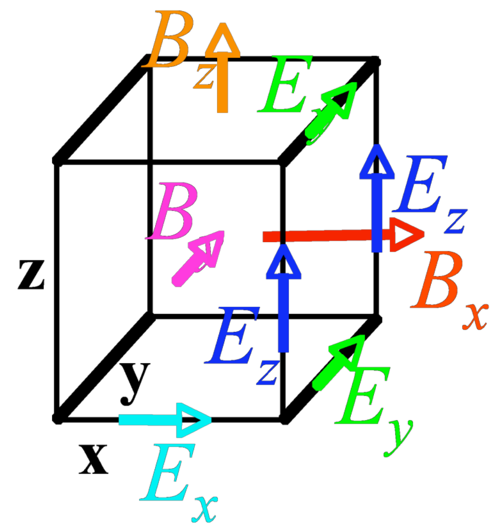
- Compute properties of EM structures (cavities, waveguides, couplers) prior to build (cost savings) as part of the design cycle
  - R/Q (acceleration/stored energy)
  - Magnetic hot spots (quenching, heat load)
  - Mode frequencies, separation
  - Multipactoring
- Optimize cavity characteristics
  - Optimization loop with above characteristics weighted
- Provide cavity characteristics for feeding into full-accelerator modeling
  - Map parameters for tracking studies
  - Heat loads

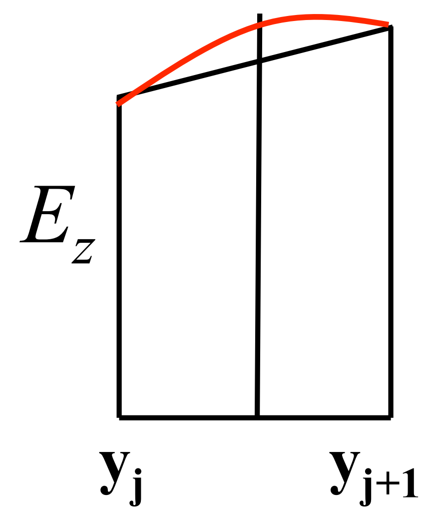
Today: show examples

FDTD computations are based on the simple, fast Yee algorithm

- No matrix inversions
- Manifestly stable
  – Symmetric update matrix
- Works well with particles (PIC)
  – The choice of PIC codes
- Parallelizes well
  – Only boundary information exchanged between domains

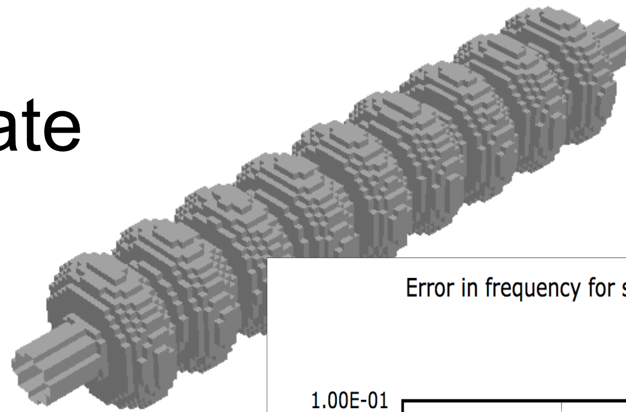
– Higher-order versions exist

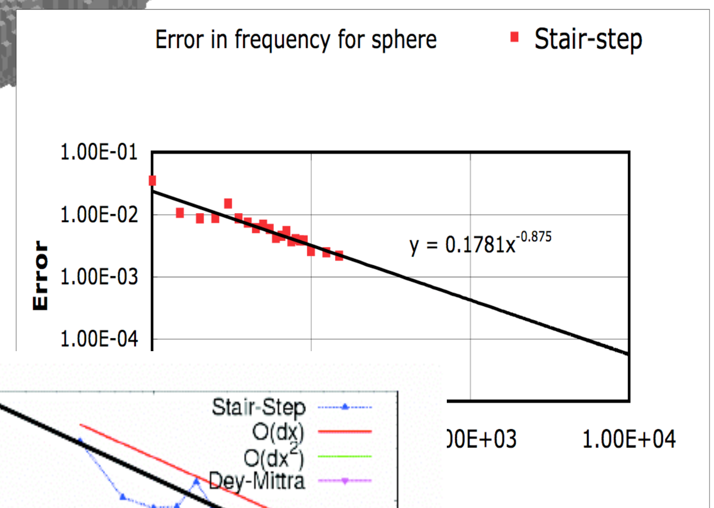


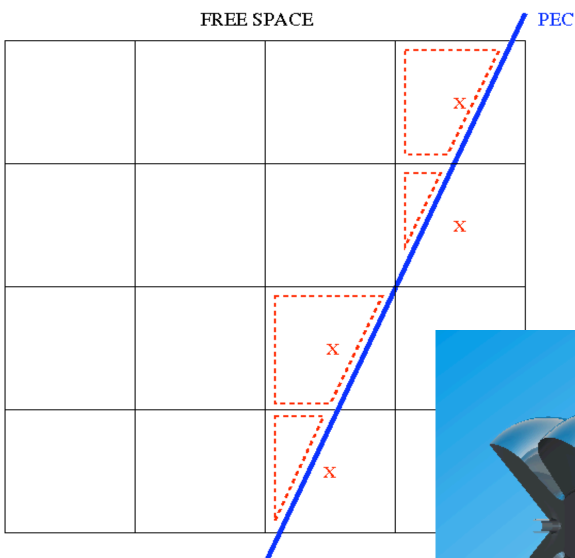


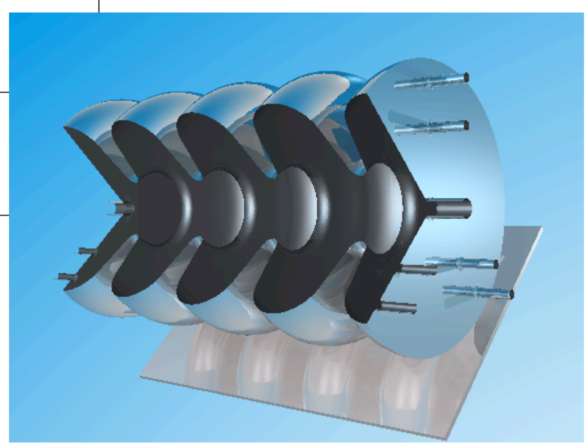
Curved structures accurately modeled with embedded boundaries

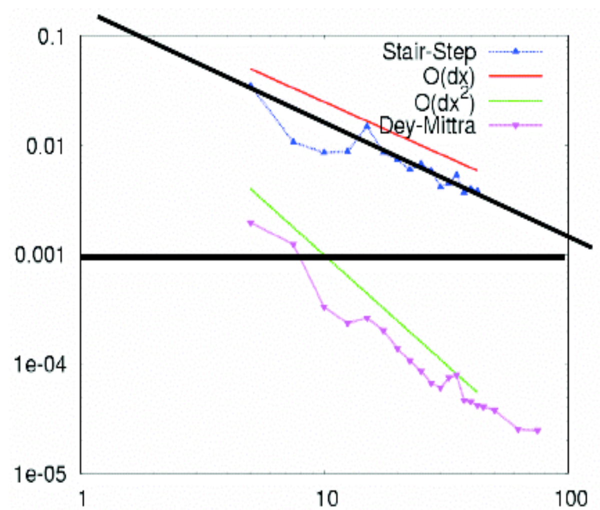
- Stairstep was not accurate
- Dey-Mittra found to give sufficient accuracy











Under SciDAC, improved algorithms found

- *Broadly filtered diagonalization method*

IER Journal of Computational Physics 227 (2008) 5200–5214

www.elsevier.con

Extracting degenerate modes and frequencies from time-domain simulations with filter-diagonalization [q]

Gregory R. Werner [a,*], John R. Cary [a,b]

[a] Center for Integrated Plasma Studies, University of Colorado, Boulder, CO 80309, United States
[b] Tech-X Corporation, Boulder, CO 80303, United States

Received 22 May 2007; received in revised form 20 December 2007; accepted 27 January 2008
Available online 5 February 2008

- *Symmetric dielectric update algorithms*

Journal of Computational Physics 226 (2007) 1085–1101

www.elsevier.c

A stable FDTD algorithm for non-diagonal, anisotropic dielectrics [q]

Gregory R. Werner [a,*], John R. Cary [a,b]

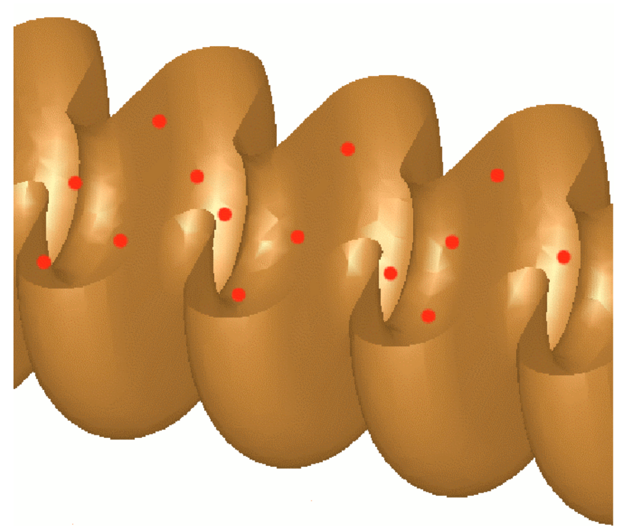
[a] Center for Integrated Plasma Studies, University of Colorado, Boulder, CO 80309, United States
[b] Tech-X Corporation, Boulder, CO 80303, United States

Received 9 February 2007; received in revised form 4 May 2007; accepted 7 May 2007

Synergy with other programs critical: SBIR, CU program

Broadly filtered diagonalization: time-domain codes become frequency domain

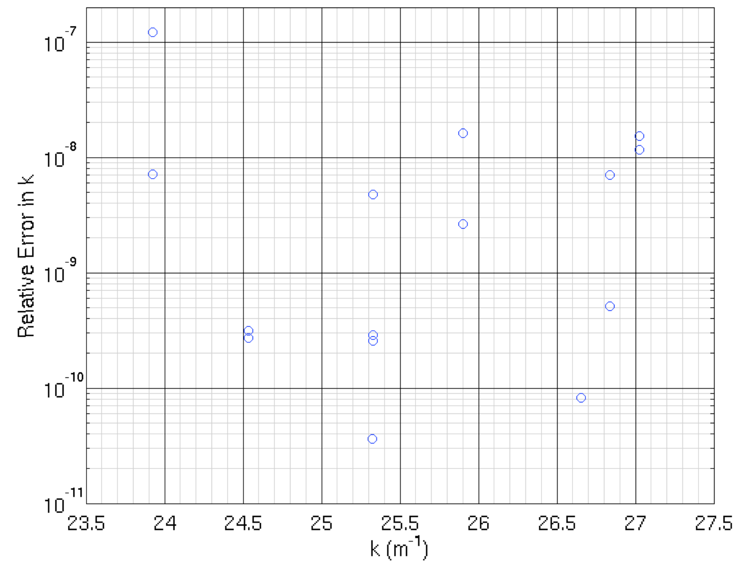
- Cavity ringing is traditional method for getting frequencies from time-domain codes
  - Excite one mode with narrow band
  - Measure FFT peak or zero crossing
  - Cannot distinguish degeneracies
- Broad filtering
  - Excite collection of modes in a frequency band
  - Collect data on a subspace
  - One application of operator gives small relative eigenvalue problem
  - Singular value decomposition determines the linearly independent subspace
  - Degeneracies found



Eliminates requirements for retention of multiple eigenvectors for eigenvalue solving

Degeneracies obtained by running multiple simulations

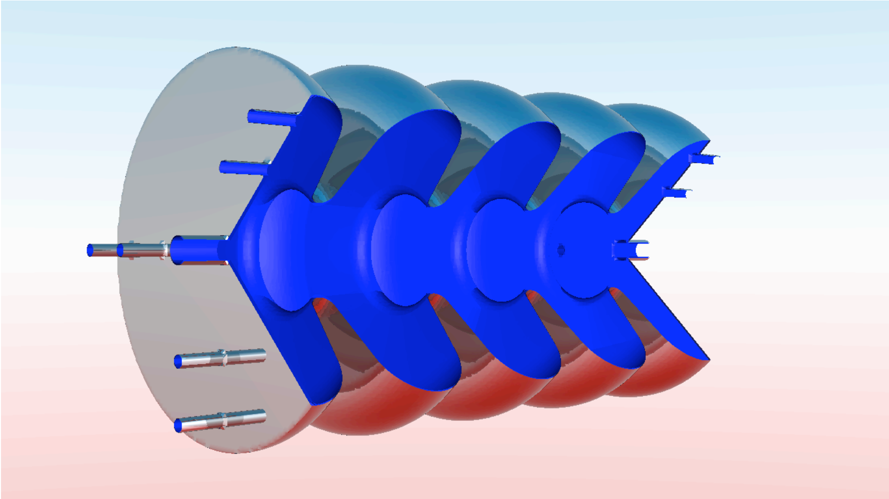
- Two modes with nearly same frequency evolve nearly identically, subspace has one linear superposition of modes
- Second simulation with different excitation gives different linear superposition.
- Combined subspace has both combinations, subspace diagonalization gives both

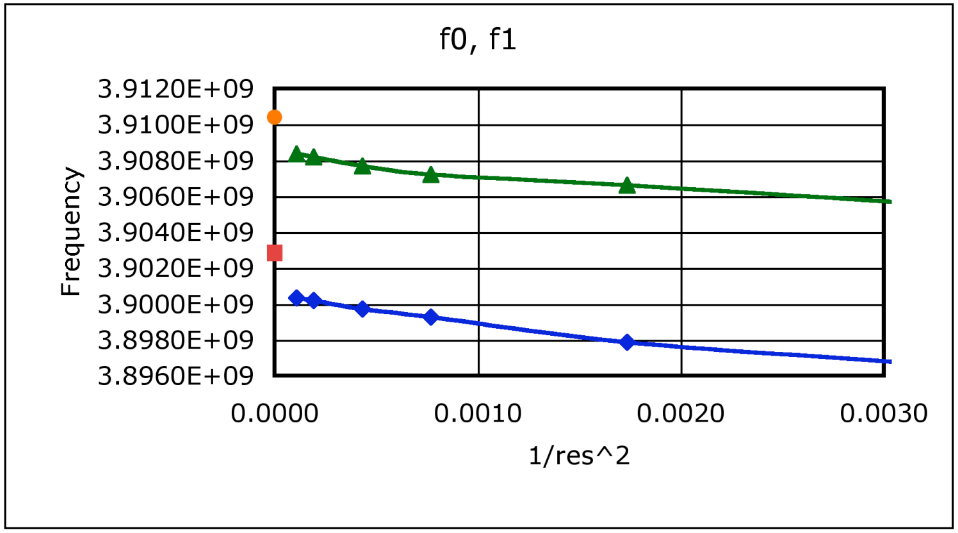


Slightly unequal square cavity, Lx =1, Ly=1.00001. Degenerate modes found.

Prior to embarking on physics studies, need to do validation

- A15 cavity for Kaon separator
- Previous computations gave frequencies low by 5 MHz out of 4 GHz.
- Ours (improved algorithm and parallelism) were low by 2 MHz, yet we had verified against exact solutions!
- Model no holes? One? All?
- Correct for dielectric of air

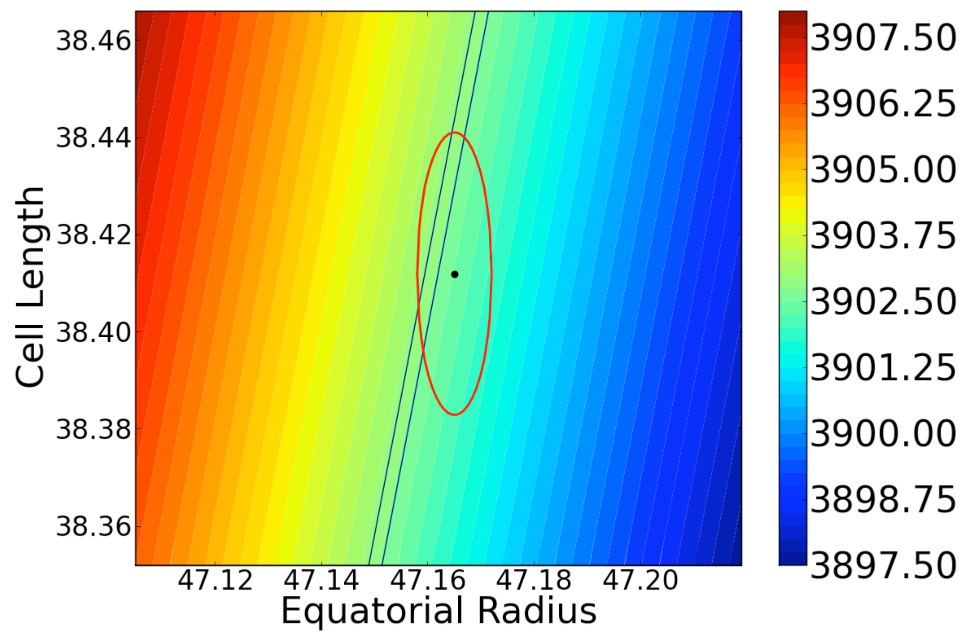




The validation study showed that we had been given the wrong model

- Reduce the equator radius by 0.001 inch
- Get agreement
- Ask designers to measure their cavities
- CORDEX (+ calipers) show error in cavity dimensions
- Corrected model agrees well with computation.

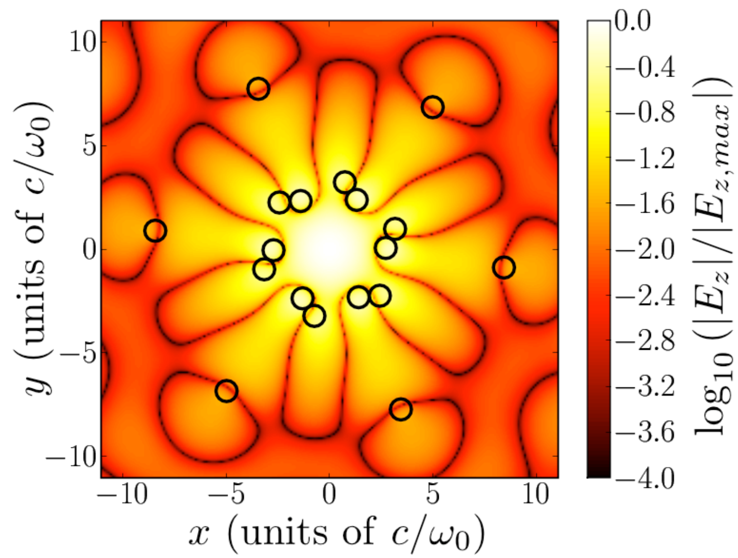
Frequency contours in cavity parameter space



Overlap of dimensional error ellipse with computational and experimental frequency uncertainty shows validation

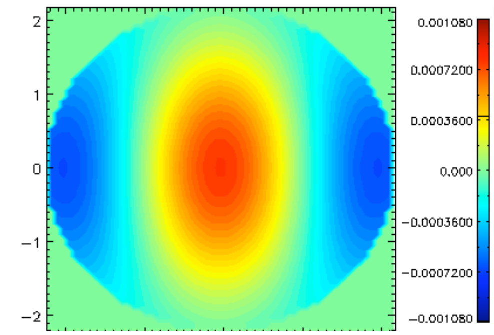
EM modeling using VORPAL in a number of areas

- Conventional cavity studies
  - Cavity map extraction
  - Multipactoring
- Photonic structures
  - Improved structures requiring many fewer rods
- Photocathode guns
  - Diamond amplifiers
- (LWFA heard from later)



Cavity maps facilitate large-scale modeling

- Compute accelerating mode using broadly filtered mode extraction
- Use those modes, on a cylindrical boundary, with vector Helmholtz equation to determine gradients on axis
- Taylor expansion gives truncated power series map for tracking studies
- RF Map used in MaryLie Impact (Synergia soon)
- Have also done dipole mode.



PHYSICAL REVIEW SPECIAL TOPICS - ACCELERATORS AND BEAMS **9**, 052001 (2006)

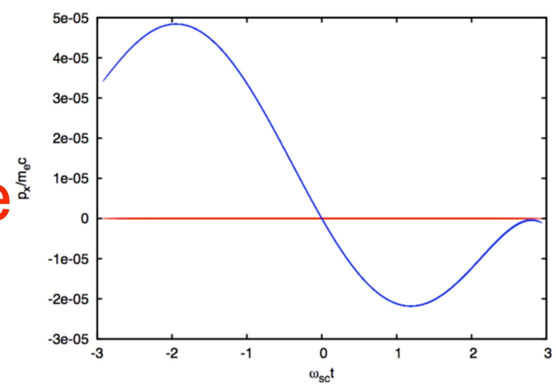
Numerical computation of high-order transfer maps for rf cavities

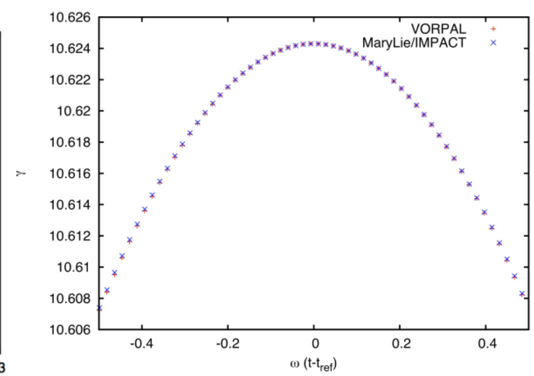
Dan T. Abell*

Tech-X Corporation, 5621 Arapahoe Avenue, Suite A, Boulder, Colorado 80303, USA

(Received 18 November 2005; published 9 May 2006)

Modern map-based accelerator beam-dynamics codes model magnetic elements so as to include nonlinear effects and realistic fringe fields, but they persist in modeling rf cavities as either energy kicks or linear maps. This work presents a method for including the nonlinear effects of rf cavities in a map-based code.





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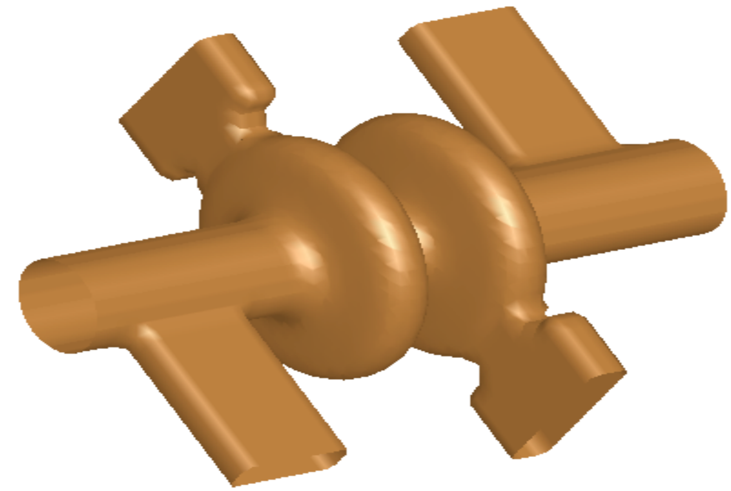
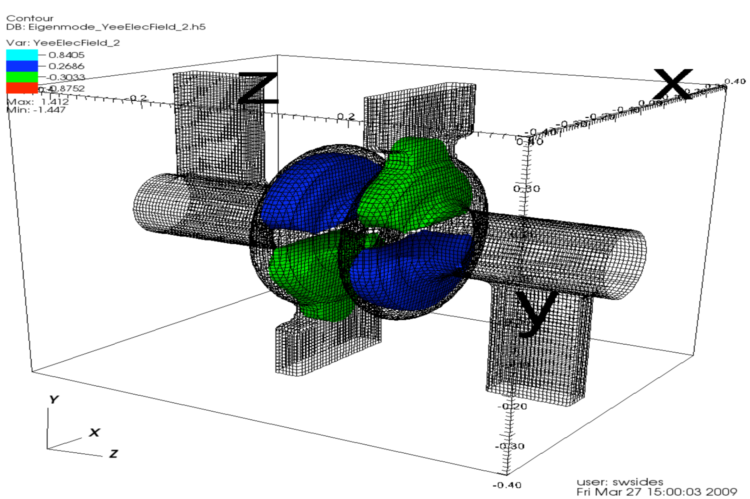
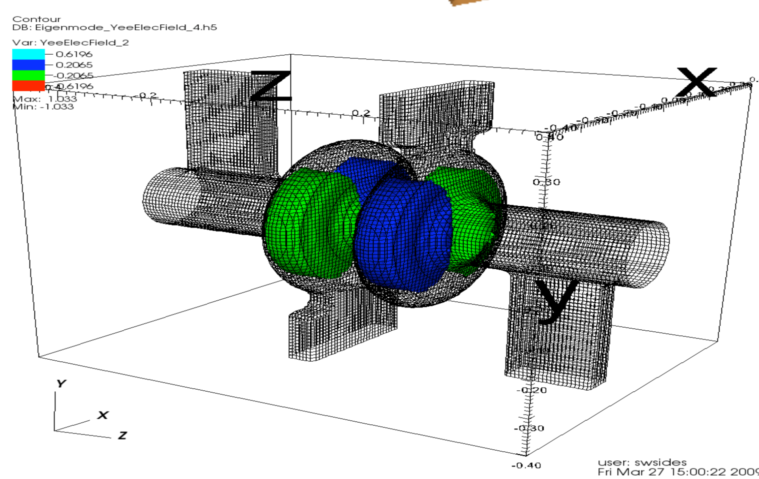
Multipactoring determining limits of crab cavities

- LHC upgrade: introduce crab cavity to improve luminosity
- Jlab/Cockcroft splitting from waveguide replacement







G. Burt, J. Smith (Cockcroft Institute)
H. Wang, K. Tian, R. Rimmer (Jefferson Lab)

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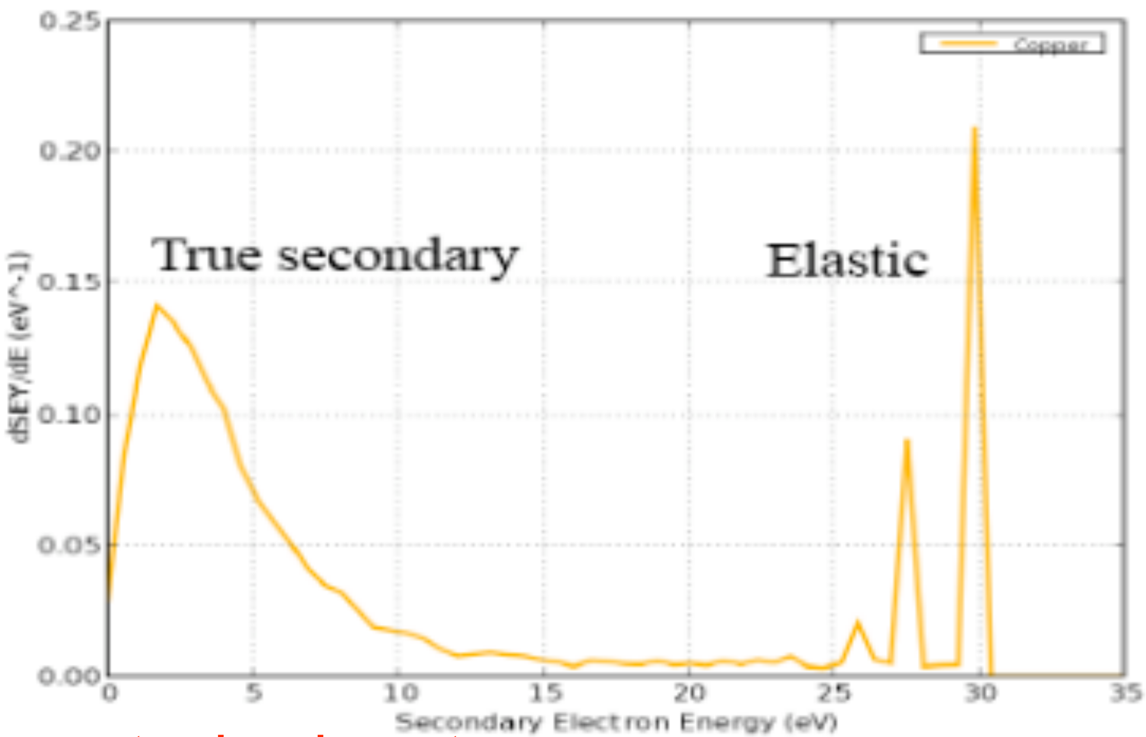
VORPAL's secondary electron emission models allow realistic multipacting studies

- Simple secondary emission – one secondary emitted at normal incidence
- Phenomenological model – true, diffuse and elastic secondaries
- M. A. Furman and M. Pivi, Phys. Rev. ST Accel. Beams 5, 124404 (2002)



Available as txphysics at http://www.txcorp.com/technologies/TxPhysics/

Library funded under SBIR. Made available in SciDAC codes.

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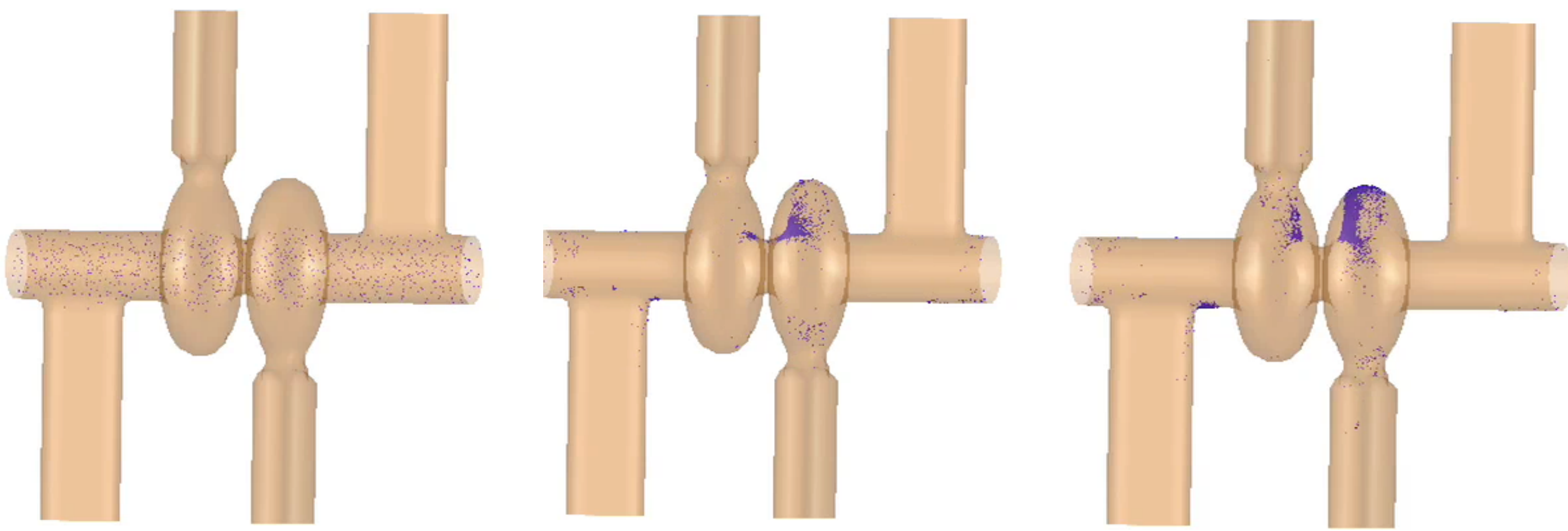
Preliminary simulations show possible multipacting in UK crab design

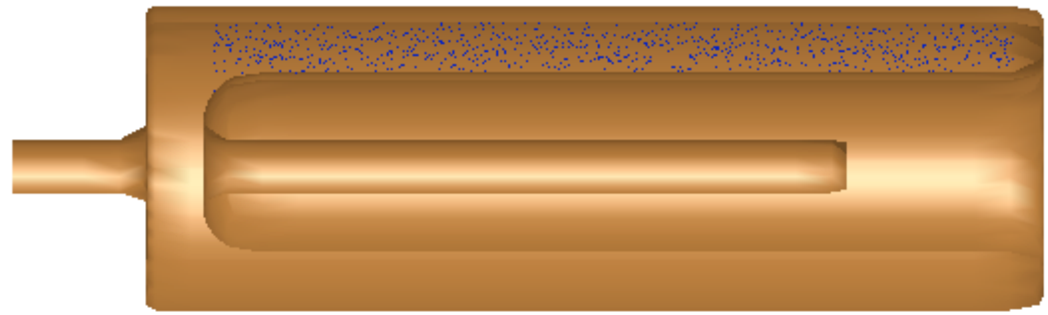
- E_{peak} ~10 MV/m
- Movement towards equator implies soft barrier multipacting

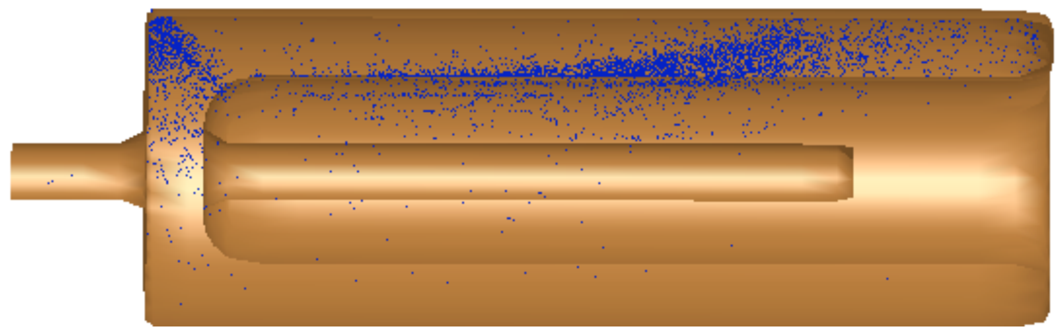


Seed electrons | Multipacting | Multipacting drift

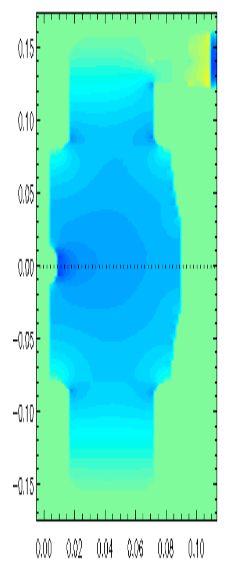
Multipacting evaluations for NP: BNL 56 MHz structures

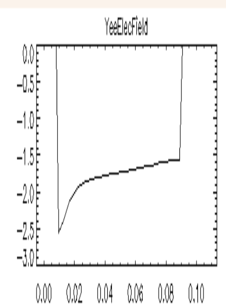
- Proposed to add 56 MHz SRF cavities for RHIC upgrade in 2011
- Seed electrons
- Multipactoring
  - Diagonal multipacting found
- Next steps:
  - Feedback into optimization loop

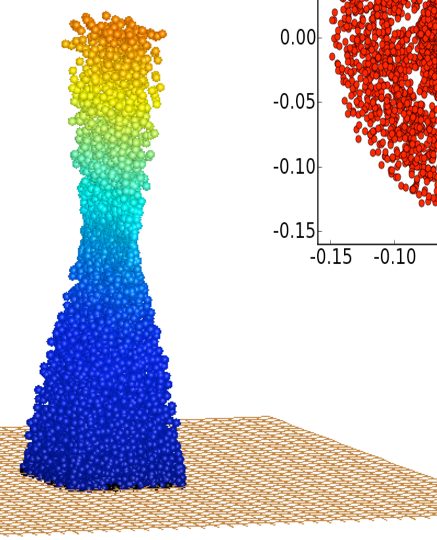


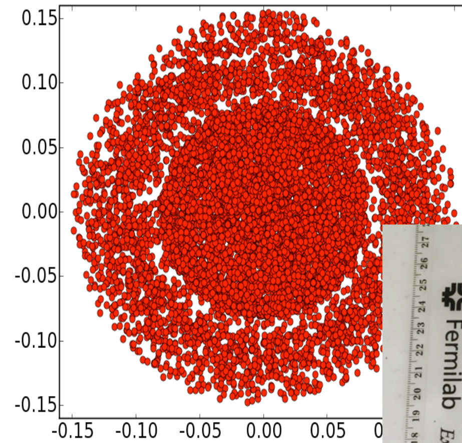


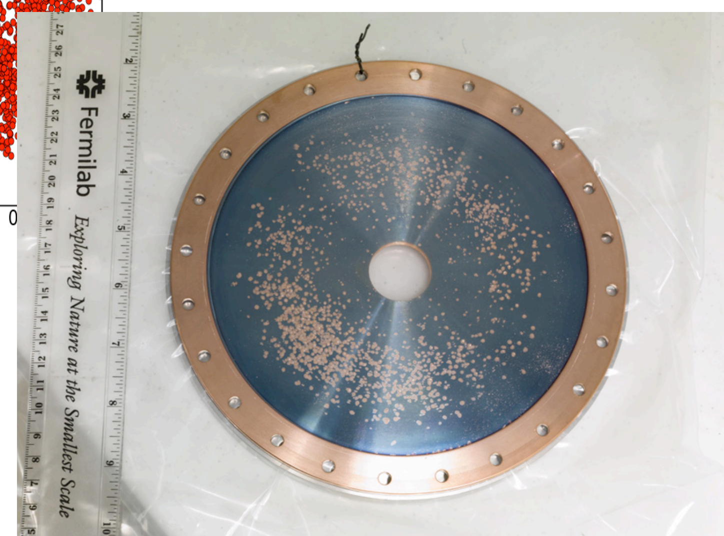
Multipacting analysis capability used to evaluate high-gradient muon collider cavities











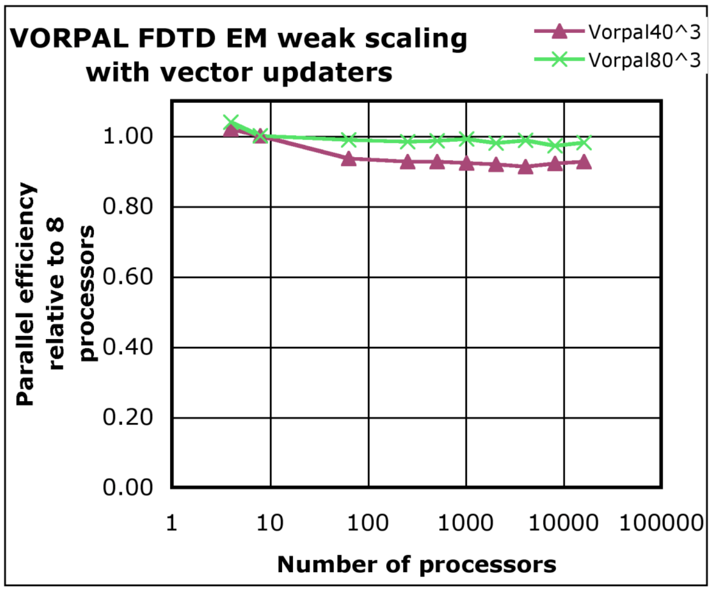
- VORPAL has accurate field models and physics-based surface emission algorithms (right)
- Multipacting and breakdown often coincident. Simulation shows multipacting where experiment shows breakdown.

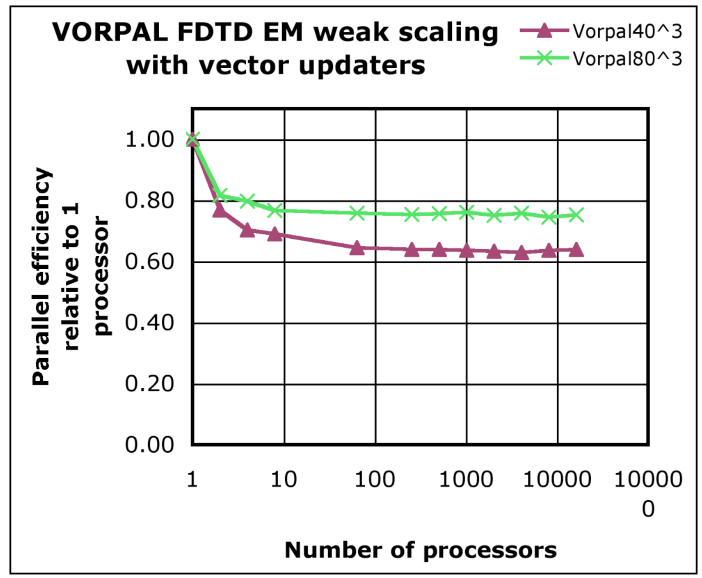
Broad usage at LCFs
(at all machines at NERSC, ALCF)

- VORPAL openly available to DOE collaborators at NERSC (thx to Katie Antypas), ALCF (no account at OLCF)
- Large number of users
  - 30 at NERSC under 5 different projects (repos)
  - 5-10 at ALCF under 2 different projects
- Large number of hours
  - NERSC: 6M hrs 2008, 2M by mid March for 2009
  - ALCF: 15M hrs 2008, 5M by mid March for 2009
- High concurrency (routine use at high processor counts)
  - NERSC, 2009: 8656 for average job
  - ALCF, 2009: 8192 cores typical

Achieving good scaling in FD EM updates

- Only surface to volume, so scales well if a domain is large enough
- (Bruhwiler will cover PIC scaling in LWFA talk)





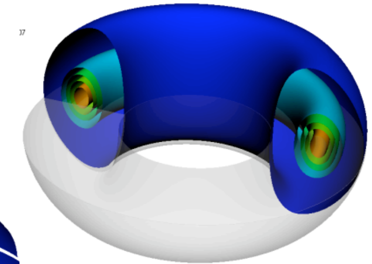
- Not strong or weak, but what does one lose going parallel?

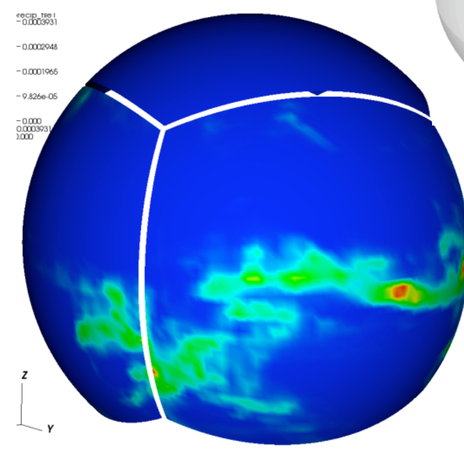
Interactions with CETs: Viz, Solvers,

- Close interaction with VACET
  - Learning VisIt
  - Teaching VisIt
  - Collaboratively writing plugins for VisIt
- Additional interactions with TOPS
  - Trilinos used for VORPAL implicit computations
- Close interactions with NERSC to determine reasons for parallel I/O problems at large processor counts (Talk given at hdf5 workshop at NERSC on Jan 20, 2009)
- Coming interaction with ITAPS
  - New postdoc to work with Tautges
  - Rapid boundary analysis
  - Higher-order embedded boundaries

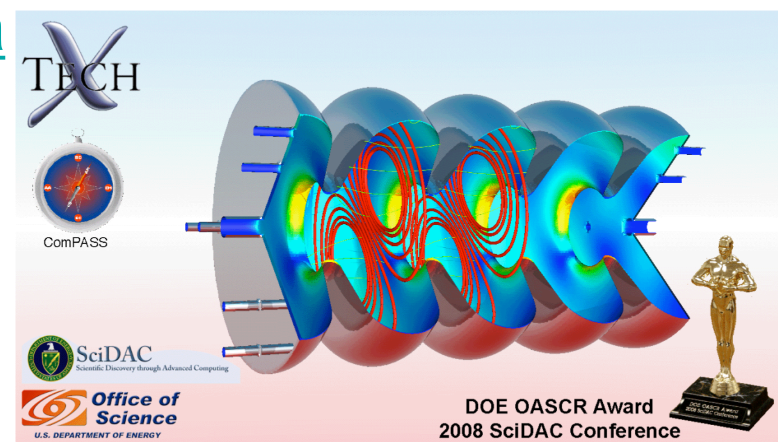
Slide from Tim Tautges

Interaction with VACET led to broad visualization capability



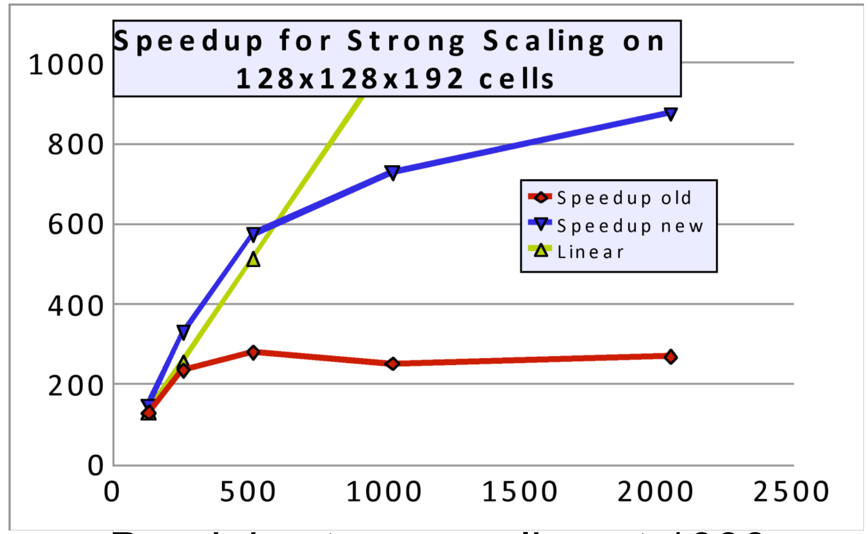


- HDF5: a "self-describing" file format
  - Can add attributes to files for describing contents
  - What are the minimal attributes needed for visualization?
- VizSchema: a schema for how to mark up data for visualization
  - Data and the
  - Meshes of the data
- https://ice.txcorp.com/trac/vizschema
- Combining domain scientists with computer scientists leads to general results



Developing: improved messaging for parallel performance enhancement

- Improved messaging: send only what is needed for FDTD
- Allows use of domains with only 3000 cells (before, 64000 cells)
- Consequences:
  - Time to solution increases by 20x if resources are available
  - Smaller problems can be addressed with high-performance computation



Break in strong scaling at 1000 procs or 3000 cell domains

- 120M cells can take advantage of 40k procs

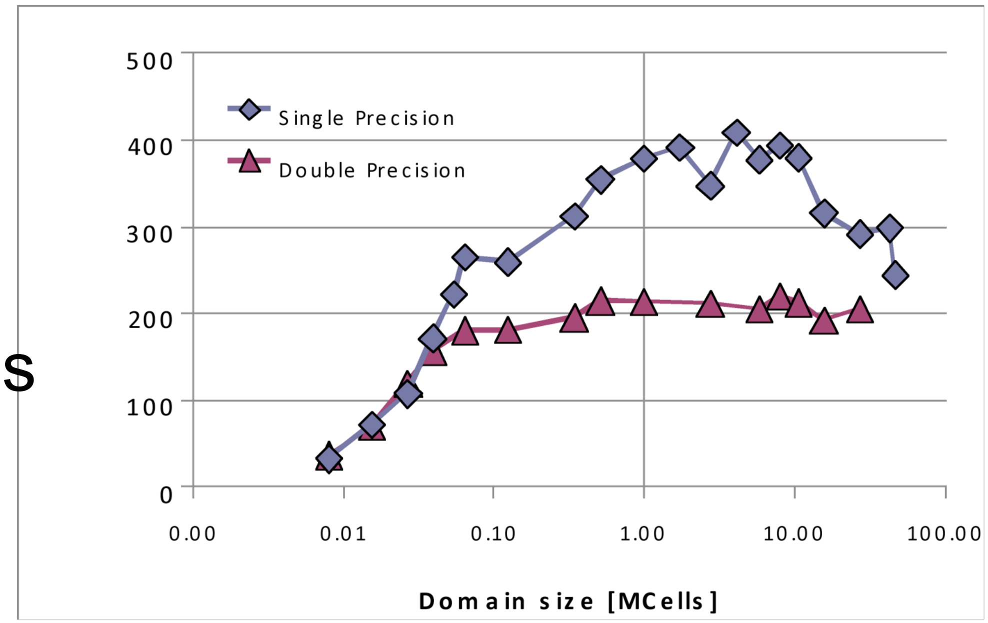
Peter Messmer[1], Ben Cowan[1], George Bell[1], Keegan Amyx[1], Boyana Norris[2], John R. Cary[1]

[1]Tech-X Corp., [2]Argonne National Lab.

Work supported by DOE ASCR SBIR Phase II DE-FG02-07ER84731 and by VORPAL customers

Developing: Improved single-processor performance using GPUs

- Many-core, lots of simultaneous threads
- Written in high-level language using GPUlib (gpulib.txcorp.com)
- Using conformal boundaries for accuracy (VORPAL generated mesh)
- Roughly 40x speedup in single, 20x speedup in double



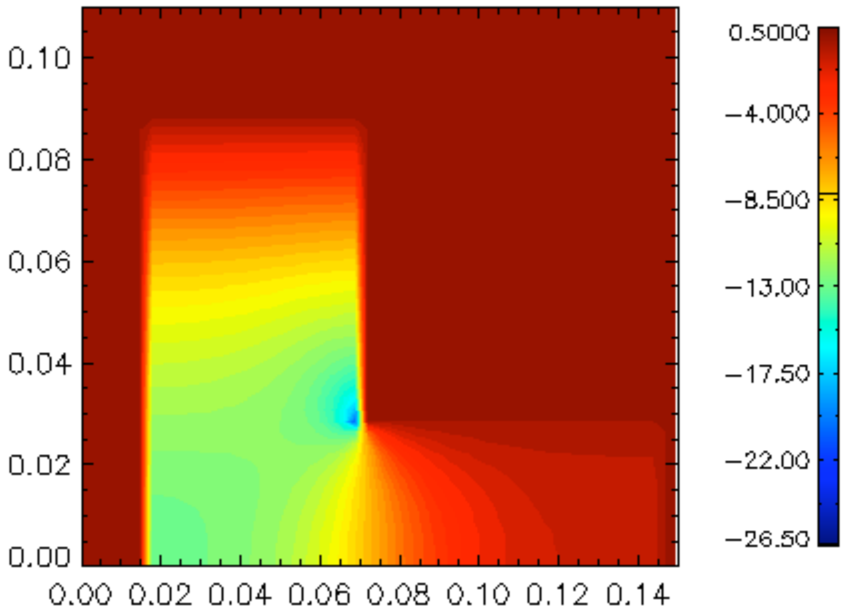
Peter Messmer, Travis Austin, John R. Cary, Paul Mullowney, Keegan Amyx, Mike Galloy

Tech-X Corp.

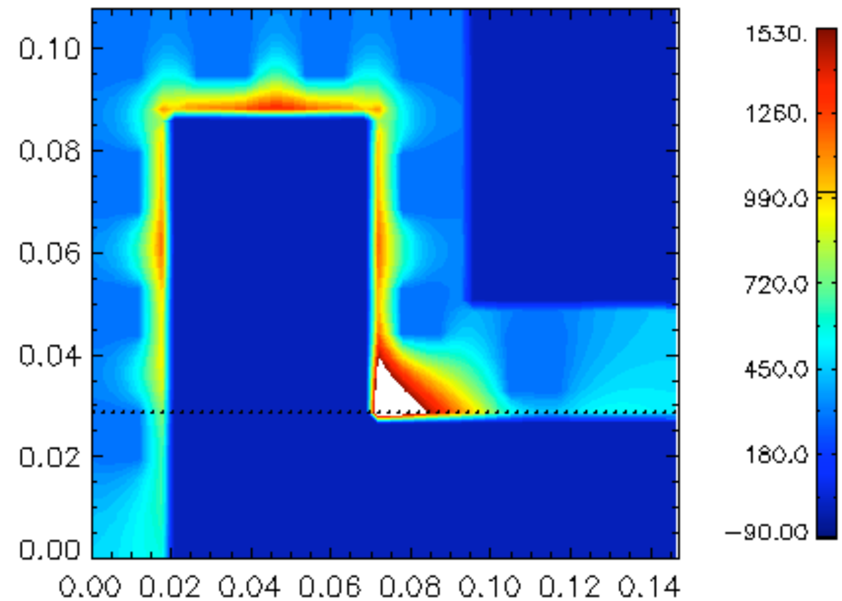
Work partially supported by NASA SBIR Phase II Grant #NNG06CA13C, NVIDIA Corp. and Tech-X Corp.

Developing direction: combined EM and heat flow

- Cartoon Photocathode Gun, with 10 coolant channels.
- “Multifield” capability permits EM and Thermal, even in same run.
- Here, thermal timescale is artificially speed-up to EM time-scale.
- Ohmic wall losses communicated between EM and Thermal.
- R_s, k, and C are temperature dependant, e.g., non-linear.



EM: E_z Electric Field



Thermal: Temperature

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Many potential developments (collaborative with OASCR)

- Ease-of-use tools for EM simulations
- Visualization
- Performance improvements
  - GPUs for EM, PIC
  - Improved messaging
- Embedded boundary developments
  - Higher-order embedded boundaries
  - Eliminate stable time step reduction
  - Particle motion near boundaries

Extra slides

Higher-order embedded boundaries would make a large impact

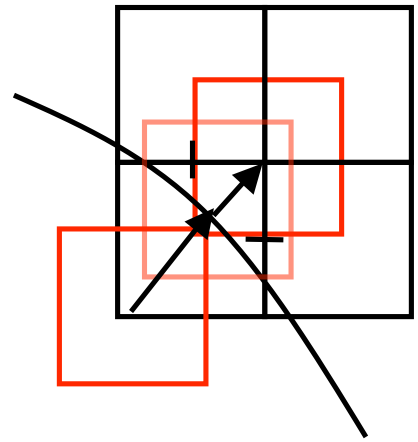
- Boundary error same as interior
  - Boundary error is $O(\Delta x)$, gives $O(\Delta x^2)$ globally
  - Interior error is $O(\Delta x^2)$
- With Richardson extrapolation
  - Boundary error is $O(\Delta x^2)$, gives $O(\Delta x^3)$ globally
  - Interior error is $O(\Delta x^4)$
- Boundary error is limiting with extrapolation
- Improved boundary error will lead to overall error of $O(\Delta x^4)$!
- We now have a derivation of Dey-Mittra
- Have higher-order algorithm, but
  - Very complex
  - Not manifestly symmetric

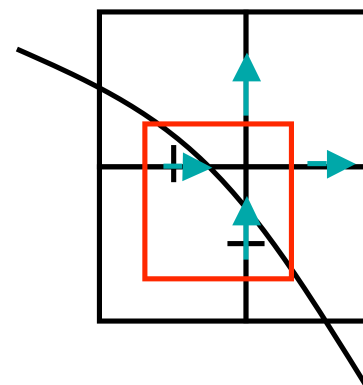
Elimination of time-step reduction improves modeling

- Reduces work by a factor of 4-10
- Eliminates spurious trapped high-frequency modes (important for multipactoring studies)
- I. A. Zagorodnov, R. Schuhmann, T. Weiland, [*A uniformly stable conformal FDTD-method in Cartesian grids*, Int. J. Numer. Model., 16, 127 (2003)] has heuristic approach based on area borrowing.
- Can one prove the above?
- Understand how to have minimal impact?
- How is symmetry imposed?

Particle dynamics near boundaries critical for accurate modeling

- Charge conservation near boundaries critical to avoid nonphysical charge buildup
- What does one do with dynamics? Without some care, we have observed self forces and excess heating.
- We are approaching heuristically: copy over
- Does this avoid self forces?





Visualization and code comparision

- Visualization what one is solving is a great aid
- For verification, would like to have easier ways to compare results
  - Exchange standards for data, geometries
- Ultimately, solve different problems and have increased productivity

2008 sample publications
(https://ice.txcorp.com/trac/vorpal)

JOURNAL ARTICLES

- N. Xiang and J. R. Cary, "Second harmonic generation of electron Bernstein waves in an inhomogeneous plasma," Phys. Rev. Lett., 100, 085002 (2008); doi:10.1103/PhysRevLett.100.085002; http://link.aps.org/abstract/PRL/v100/e085002.
- Karoly Nemeth, Baifei Shen, Yuelin Li, Robert Crowell, Katherine C. Harkay, and John R. Cary, "Laser driven coherent betatron oscillation in a laser-wakefield cavity," Phys. Rev. Lett. 100, 095002 (2008), doi:10.1103/PhysRevLett.100.095002, http://link.aps.org/abstract/PRL/v100/e095002.
- G. R. Werner and J. R. Cary, "Extracting Degenerate Modes and Frequencies from Time Domain Simulations," J. Comp. Phys. 227, 5200-5214 (2008), http://dx.doi.org/10.1016/j.jcp.2008.01.040.
- C.G.R. Geddes, K. Nakamura, G.R. Plateau, Cs. Toth, E. Cormier-Michel, E. Esarey, C.B. Schroeder, J.R. Cary, and W.P. Leemans, "Plasma density gradient injection of low absolute momentum spread electron bunches," Phys. Rev. Lett. 100, 215004 (2008).
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